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Geometry and Hamiltonian mechanics on discrete spaces

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Abstract

Numerical simulation is often crucial for analysing the behaviour of many complex systems which do not admit analytic solutions. To this end, one either converts a 'smooth' model into a discrete (in space and time) model, or models systems directly at a discrete level. The goal of this paper is to provide a discrete analogue of differential geometry, and to define on these discrete models a formal *discrete Hamiltonian structure*—in doing so we try to bring together various fundamental concepts from numerical analysis, differential geometry, algebraic geometry, simplicial homology and classical Hamiltonian mechanics. For example, the concept of a twisted derivation is borrowed from algebraic geometry for developing a discrete calculus. The theory is applied to a nonlinear pendulum and we compare the dynamics obtained through a discrete modelling approach with the dynamics obtained via the usual discretization procedures. Also an example of an energy-conserving algorithm on a simple harmonic oscillator is presented, and its effect on the Poisson structure is discussed.

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1. Introduction

Numerical simulations are of fundamental importance in our understanding of system behaviour. Since most complex systems do not admit closed-form analytic solutions, the only alternative in many cases is numerical simulations. Simplistically speaking, we can define numerical simulation as follows: one takes a system defined by differential (ordinary or partial) equations, performs a transformation (i.e. discretization) of the mathematical model into an algebraic setting called finite differences (i.e. difference equations), which is then implementable on computers for numerical simulation. Most of the focus in numerical

simulation has not been on preserving the *structure* of the original system model. Indeed, it is mainly from recent times that researchers have been *actively* studying what can be called *structure-preserving algorithms* [1–5]. These include conserving the symplectic structure, or energy conservation, or momentum conservation, conservation of various other first integrals etc. For example, some of the most popular algorithms for simulation of mechanical systems (such as the Newmark algorithm, which is used in nonlinear structural dynamics, and the Verlet and SHAKE algorithms of molecular dynamics) turn out to be structure-preserving variational integrators. Interestingly, this was not known at the time these algorithms were discovered; they came to be widely used because of their superior long-time behaviour (see [3] for further discussion). While such structure-conserving algorithms are gaining importance in the field of numerical simulation, there are still a few fundamental aspects that have not been studied. One issue is as follows: numerical simulation requires a smooth model to be transformed (using any of the various discretization techniques) into a *fully discrete model*, i.e. discrete in space and time. While the discretization techniques themselves have been the subject of a great deal of research, not much is known about the formal mathematical/geometrical structure of the final discrete model in relation to the structure of the smooth model. What we mean by this is, for example, suppose we have a smooth model defined in the Hamiltonian framework, and we have all the associated structure on the cotangent bundle. Let us now discretize this model; what is then the associated *discrete Hamiltonian structure*? Alternatively, one could model systems directly at a discrete level, and then again we have the same issues. This paper lays the mathematical foundations of a formal study of discrete systems from our viewpoint. The focus of the paper is on studying discrete analogues of some fundamental mathematical tools used in differential geometry. As such we start with the algebraic structure of floating point numbers: we treat this set as the discrete analogue of the reals $\mathbb{R}$, and since computers use floating point numbers for their operations we prefer to work in this set. Another issue is to understand the impact of structure-preserving techniques on the geometric structures that discrete models possess. We present an example in this paper where we show how the geometric structure changes significantly when one goes from techniques which are not structure-preserving to techniques which are.

Before embarking on our study let us try to review in brief, various related studies done in this aspect. As such, this is an incomplete review, we present only those studies that have influenced our own research. Greenspan [6] presents a discrete version of calculus based on finite differences without giving explicit attention to the algebraic properties of this calculus. His approach can be, roughly speaking, said to be a kind of 'particle' modelling approach towards the simulation of physical systems. So, for example, a vibrating string is considered to be a collection of vibrating particles, each interacting with the other via the usual Newtonian laws (similarly for fluids, gases, etc). Such a scheme is wonderfully suited for cellular automata simulations (see [7]), but as yet it is not very useful if the designer would like to have more formal structure in the system, say for example a Hamiltonian/Lagrangian structure. Next, Baez and Gilliam [8] and Gilliam [9] present an algebraic approach towards discrete mechanics in a Lagrangian framework. In short, they consider the geometric/mathematical structure defined on fields (like $\mathbb{R}^n$) of smooth systems and present algebraic analogues on more general rings. So, for example, vector fields are replaced by derivations and differential forms are replaced by Kähler differentials [10]. However, as we will argue in this paper, in the discrete setting it is not derivations that are the appropriate replacement for vector fields, rather it should be the so-called twisted derivations. Also the set of floating point numbers is a not a ring in the usual sense, so we would need to work with different algebraic structures. Also this seemingly simple idea will have non-trivial consequences when defining the Hamiltonian/Lagrangian structures.

Our goal in this paper is two-fold: firstly we present a formal calculus (and the analogue of differential geometry) on discrete spaces which in some sense can be considered as unifying, in the discrete setting, the above-mentioned studies by Greenspan [6], Baez and Gilliam [8] and Gilliam [9]. We also analyse the relation between the discrete models and the continuous ones. In this sense, we recall the notion of the tangent groupoid of a differentiable manifold and use its topological structure to justify the limit process of a series of discrete models defined on discrete spaces (i.e. defined by floating point numbers) tending to a smooth one if we consider the precision of the computer approaching infinity (in other words, taking the natural continuum limit of floating point numbers). Once the tangent groupoid is used to define the notion of a discrete vector, we define the rest of the ingredients required to define an analogue of the usual smooth calculus, discussing the main differences arising in the discrete world. Then, mimicking the definition of smooth Hamiltonian mechanics, we develop a discrete Hamiltonian mechanics and discuss what energy conservation would mean with regards to the 'discrete' geometric structure. The other goal is to use the framework of this paper as the building block towards understanding how the concept of discrete Port-Hamiltonian systems [11] can be used to derive a new geometric setting for the numerical simulation of Hamiltonian systems, this work [11] is currently in progress. Also we discuss more of this in section 7.

The paper is organized as follows: in section 2 we give a short summary of the algebraic structure of floating point numbers $\mathbb{F}^n$; see [12, 13] for more details. Then in section 3 we define a discrete (local and global) calculus on $\mathbb{F}^n$, where the concept of a twisted derivation is employed. In section 4 we show the relationship between various integration techniques and discrete vectors, and we discuss the concept of discrete differentiability. Section 5 introduces discrete manifolds and, finally, in section 6, we define discrete Hamiltonian mechanics and show an important relationship between the discrete Poisson structure and energy-conserving algorithms.

2. The algebraic structure of the set of floating point numbers

Differentiable manifolds locally look like Euclidean $\mathbb{R}^n$. If we want to extend this definition to more general manifolds, we need to replace the field $\mathbb{R}$ by a general ring. In the case of discrete manifolds, defined later on, we would like to replace $\mathbb{R}$ with the set of floating point numbers $\mathbb{F}$. The reason for this is very simple; since most computers work with floating point numbers, from our point of view this is the most obvious choice. However, unlike $\mathbb{R}$, $\mathbb{F}$ does not have an algebraic structure—as one usually understands it. $\mathbb{F}$ is a finite set, and algebraic operations defined on $\mathbb{F}$ usually have results that are truncated (because of the finite precision of floating point numbers [14, 15]), and hence some of the basic algebraic properties like associativity and distributivity are destroyed. Hence $\mathbb{F}$ is *not even a ring* (cf [12, 15] for more details), and then it seems that there is simply no way that we can use it as a replacement for $\mathbb{R}$ in the discrete setting. However, since we would like to extend the concepts of differential geometry to the discrete setting, we have to endow $\mathbb{F}$ with some *new* algebraic structure.

The properties of floating point numbers have been very well researched (cf [14, 15] among others). For the purpose of studying discrete mechanics the algebraic structure of the set of floating point numbers is straightforward to deal with. The algebraic structure is itself quite simple. $\mathbb{F}$ is an example of what is called a *quasi-ring* (cf [12]). Loosely speaking, a quasi-ring (like $\mathbb{F}$) is a *finite* set closed under two special operations denoted by $+, \cdot$ s.t. in general the set does not have the associativity and distributivity properties of ordinary rings. The terminology 'quasi-ring' is quite appropriate, since in the continuum limit of quasi-rings (like $\mathbb{F}$), i.e. as we add more and more points to $\mathbb{F}$, one recovers the usual ring properties of associativity and distributivity. $+, \cdot$ are called 'special' because in $\mathbb{F}$ all operations are truncated, unless they

fall within a certain finite precision range, - for example: $2 + 10^{-15} = 2$ in many computer architectures. Hence, one can loosely think of $+, \cdot$ being the usual operations in $\mathbb{R}$ followed by a truncation process.

Example 1. Floating point numbers $\mathbb{F}$ are examples of quasi-rings. The properties[3] of the set of floating point numbers are

Closure under addition and multiplication	Yes
Associativity/distributivity of addition and multiplication	No
Additive and multiplicative commutativity	Yes
Unique identity element w.r.t. $+, \cdot$	Yes
Unique additive and multiplicative inverse	Yes

Hence $\mathbb{F}$ is a quasi-ring, this will be our discrete analogue of the reals (which is a field, i.e. a ring with a multiplicative inverse). In our approach, space and time are considered as discrete, and importantly our system variables take their values in $\mathbb{F}$, the same holds for the independent variables space and time. So for example systems do not evolve in integer time steps, rather they evolve in floating-point time steps.

The point spacings in $\mathbb{F}$ are not constant, and it is in this respect that our approach is fundamentally different from the usual lattice approach to discretization. Both from a mathematical and a physical point of view[4], it is important to not be restricted by 'regular' lattices. We will argue in this paper certain mathematical limitations to the use of regular lattices.

It is important that whatever discrete structure we define on $\mathbb{F}$, must in the continuum limit go to the correct smooth analogues. Hence, before developing such discrete structures, we first take a look at the continuum limit properties of $\mathbb{F}$ itself.

3. Non-regular lattices

In the formulation of discrete mechanics the underlying space (on which the physical system evolves) has usually been assumed to be a lattice. For an algebraic exposition of this topic one can refer to [8]. The use of lattices has been most heavily researched in the physics community (especially in QCD studies); a good reference is [16]. We are interested in modelling mechanical systems at the discrete level in order to be able to represent those models on a computer. We require discreteness because computers are not able to represent continuous variables, since they can only handle floating-point numbers. The set of floating-point numbers $\mathbb{F}$ is quite 'similar' to regular lattices, but it exhibits an important difference: *the spacing between two consecutive elements is not constant*. There are certain limitations to the use of lattices for modelling physical systems—one has problems with the continuum limit interpretation, see remark 1; also lattices do not have, for example, full rotational symmetry and this is a serious limitation for a discrete physical theory (see [17]). Floating-point spaces also do not have full rotational symmetry. But because they do not have a regular structure like lattices, it may be possible to modify the definition of the spatial structure (by making the

[3] Note that the properties of $\mathbb{F}$ are not being defined formally. The reason for this is that these properties are very well known, and one would need to introduce many entities in order to formally define this, which we cannot do due to space constraints. In [12] we have formally defined quasi-rings and the properties of $\mathbb{F}$.

[4] As a simple example, in the simulation of waves with turbulence, in the regions of turbulence, one would like to have smaller point spacings so as to capture the turbulence effects more accurately and to have larger point spacings in regions where nothing much of interest happens. This is the physical motivation for choosing different point spacings in $\mathbb{F}^n$.

points behave in a stochastic manner, just the way that cellular automata particles are made to behave) and then one might be able to recover the correct symmetries. However this is not at all evident at the moment. But it is our opinion that floating-point spaces offer the best possibility for such a venture. Let us now revisit floating-point numbers from a slightly different viewpoint.

Definition 1. *A floating point number corresponds to a sequence of bits in the form*

$$SE\cdots EF\cdots F \Longrightarrow (-1)^S \times 1.F\cdots F \times 2^{E\cdots E-B},$$

where S determines the sign (as $(-1)^S$*), E* $\cdots$ *E represent the exponent, which is biased by B to allow negative values, and F* $\cdots$ *F represent the mantissa which fixes the precision.*

Compared to the real numbers, $\mathbb{F}$ is not dense, but yet the variation (in the point spacings) is not random, since it depends on the range of numbers represented by the exponent. Hence, for numbers with the same value of the exponent, the spacing is constant and equal to 2^{e-n_m} where e is the value of the exponent and n_m is the number of digits of the mantissa. It is easy to see:

Lemma 1. *The set of floating-point numbers is only continuous for a representation with an infinite number of bits in the mantissa.*

A very important issue to be taken into account is that the cardinality of the set of floating point numbers depends on the computer we work on: the larger the memory, the larger and denser the set. Therefore, continuum limit is also a natural goal in the process.

In this sense, we can write:

Lemma 2. *Consider the floating-point numbers space with a varying number of digits N, and denote the resulting set as* $\mathbb{F}_N$*. Then, the limit when* $N \to \infty$ *are the real numbers, i.e.* $\lim_{N\to\infty} \mathbb{F}_N = \mathbb{R}$.

As we are interested in modelling physical systems, it is enough to be able to recover a subset of the reals $\mathbb{R}^n$, which, without loss of generality, can be considered to be $V = [0, 1)^n \subset \mathbb{R}^n$. Henceforth we drop the subscript N from $\mathbb{F}_N$ unless we explicitly need to use it.

Definition 2. *Consider a* non-regular discrete space $\mathbb{F}^n$ *to be any discrete set of V such that, for any two consecutive points in one direction, the Euclidian distance between them is an element of* $\mathbb{F}$.

Obviously, the cardinality of the set $\mathbb{F}_N$ corresponds to the number of real numbers which can be defined by using N bits in the representation. It is exactly 2^N, as in the case of the integers.

Definition 3. *Let A and B be two discrete spaces. We shall call* discrete mapping *any bijection between the sets* $\Psi : A \to B$.

Asking the discrete mapping to be a bijection only is not sufficient; for example in the smooth setting one asks for differentiability also. In fact, in our discrete setting we demand the discrete mapping to be also *discrete-differentiable*, a concept we introduce in section 4.2.

3.0. A 'basis' for $\mathbb{F}^n$

In the following, it will be quite useful to define the analogue of basis for floating point numbers. It is trivial to see:

Lemma 3. *The elements* $(\overbrace{(1,0,\ldots,0)}^{n},\overbrace{(0,1,0,\ldots,0)}^{n},\ldots,\overbrace{(0,\ldots,0,1)}^{n})$ *generate the elements in* $\mathbb{F}^n$ *with linear combinations of* $\mathbb{F}$ *elements. We will refer to this as the* canonical set of generators *or* canonical basis *of* $\mathbb{F}^n$.

Proof. In each dimension, the property is trivial, since the value of the element of $\mathbb{F}$ itself defines the suitable coefficient, i.e.

$$(\lambda_1,\ldots,\lambda_n)=\lambda_1(1,0,\ldots,0)+\lambda_2(0,1,0,\ldots,0)+\cdots+\lambda_n(0,\ldots,0,1),\quad \lambda_i\in\mathbb{F}.$$

The system does not define a basis, although, because the representation is not unique. Any element $\mu_i\in\mathbb{F}$ such that $\lambda_i\cdot\mu_i=0$ (truncation errors!) allows to define a set as $(1,\mu_2,0,\ldots)$, with the same coefficients. In spite of this, with respect to this 'basis', the decomposition is unique, because the element $1\in\mathbb{F}$ is the identity element for the product. □

Note that even though we should not be using the word 'basis' (since this is meant only for vector spaces), we will stick to this abuse of terminology.

3.1. Calculus on $\mathbb{F}^n$

In this section we study a discrete analogue of calculus on what we call non-regular discrete spaces [12] (an example of such a space being the space of floating-point numbers). We argue in remark 1 why such a approach is preferable to developing a discrete calculus on regular lattices, by giving one example of a problem in the continuum limit interpretation of the lattice structure.

Our main objective is the definition of the analogue of the geometrical description of Hamiltonian mechanics on smooth manifolds. Hamiltonian mechanics defines a dynamical system on a smooth manifold by defining a vector field associated to a special function (the Hamiltonian) whose flow defines the trajectories. Then, we must define discrete dynamical systems and we intend to do it by defining discrete vector fields and a suitable notion of flow on discrete spaces. Besides, we want to obtain smooth dynamical systems as an ideal limit of our discrete systems defined as the discrete space that has an infinite number of points (or equivalently, infinite density). Therefore, we need a discrete analogue of the geometrical objects we use at the smooth level (functions, vector fields, differentiable forms, etc), which go to the corresponding smooth objects when the limit is considered. But we also need to define the limit process itself properly. We do that by using the notion of tangent groupoid below, that, at the same time, allows us to define the analogue of vectors at the discrete level, which is the basic ingredient of our discrete dynamical system.

Therefore we take the following approach to developing a discrete calculus on $\mathbb{F}^n$: firstly we define discrete functions, as a natural object for a set, then discrete vectors and discrete covectors. Using these we define global objects like discrete tensors, discrete vector fields and discrete forms. Towards the end of the section we touch upon an important aspect of our discrete mechanics—the relation between various integration techniques and different 'types' of discrete vectors. Finally we present the concept of discrete differentiability.

3.1.1. Functions. The most obvious step would be to consider functions in the natural way, i.e as mappings from $\mathbb{F}^n$ onto the elements of $\mathbb{F}$ (the one-dimensional discrete space): $A(\mathbb{F}^n) = \{f^\epsilon : \mathbb{F}^n \to \mathbb{F}\}$.

It is trivial to see that the set $A(\mathbb{F}^n)$ can be endowed with an additive structure which makes of it a group. Also we can choose as scalars the elements of $\mathbb{F}$ itself. The product by scalars is closed in $\mathbb{F}$. In any case, from the set theoretical point of view, it is trivial to see that the continuum limit of the set above becomes the set of functions of $\mathbb{R}^n$, i.e.

Lemma 4. $\lim_{N\to\infty} A(\mathbb{F}_N^n) = A(\mathbb{R}^n)$.

3.1.2. Discrete vectors: the tangent groupoid. Our goal now is to define an analogue for vectors at the discrete level. From a naive numerical approach we know that we can represent a directional derivative by using two points, defining the corresponding vector. Actually, it can be carefully proved that, from a geometrical point of view, the definition is consistent and does define a nice topological behaviour for the continuum limit. The argument is a bit technical, although, so we present a, hopefully, clear summary. More details can be found in [18, 19].

Definition 4. *A groupoid $G \rightrightarrows G^0$ consists of a set G, a set G^0 of 'units' with an inclusion $G^0 \hookrightarrow G$, two maps $r, s : G \rightrightarrows G^0$ and a composition law $G^2 \to G$ with domain*

$$G^2 := \{(g, h) : s(g) = r(h)\} \subset G \times G,$$

subject to the following rules:

(i) *if $g \in G^0$ then $r(g) = s(g) = g$;*
(ii) *$r(g)g = g = gs(g)$;*
(iii) *each $g \in G$ has an 'inverse' g^{-1}, satisfying $gg^{-1} = r(g)$ and $g^{-1}g = s(g)$;*
(iv) *$r(gh) = r(g)$ and $s(gh) = s(h)$ if $(g, h) \in G^2$;*
(v) *$(gh)k = g(hk)$ if $(g, h) \in G^2$ and $(gh, k) \in G^2$.*

In this sense, we see that a groupoid is a structure with a composition law for which there are two different units (one for the left and other for the right action) for each element. This implies that the inverse element has to produce two different results depending on the side it acts. Simple examples are the *pair groupoid* and *a vector bundle*:

Example 2. Let M be a differentiable manifold. We can define on M a groupoid very similar to the first example of the equivalence relation. This case will be helpful in the following and it is also one of the simplest cases we can find:

- The set G is $M \times M$, i.e. the point of the product manifold.
- The set G^0 is the diagonal of M, i.e. the set of points $G^0 = \{(p, p) \mid p \in M\}$.
- The projections s and r are just the projections onto the first and the second copy of M, respectively.
- The product is easily defined on $G^2 = \{((x, y), (y, z)) \mid (x, y), (y, z) \in M \times M\}$, as

$$\cdot : G^2 \to G,$$
$$(x, y) \cdot (y, z) = (x, z).$$

- Finally, the inverse element is defined as $(x, y)^{-1} = (y, x)\ \forall (x, y) \in M \times M$.

Example 3. Another interesting example for us is the case of a vector bundle $\pi : E \to M$ (in particular we will be interested in the tangent or normal bundle case).

- The set G is E, i.e. the bundle itself.
- The set G^0 is M, the base of E considered as the zero section $G^0 = \{(p, 0) \mid p \in M\}$.
- The projections s and r are both equal to the projection of the fibre bundle.
- The product is easily defined on $G^2 = \{(p, A_p)(p, B_p) \mid p \in M, A_p \cdot B_p \in \pi^{-1}(p)\}$,

$$\cdot : G^2 \to G,$$
$$(p, A_p) \cdot (p, B_p) = (p, A_p + B_p).$$

- Finally, the inverse element is defined as $(p, A_p)^{-1} = (p, -A_p)$).

We can combine both structures to define a smooth groupoid knows as the *tangent groupoid*. We define it in the most general case, which will be useful for us later, although by now we are interested only in the case of $M = \mathbb{R}^n$.

Let us prove that $G = M \times M \times]0, 1] \cup TM$ is a groupoid on $G^0 = M \times [0, 1]$, by combining the structures of the two examples above. Its components are the following

- The inclusion map $G^0 \hookrightarrow G$ is defined as

$$\begin{cases} (x, \nu) \mapsto (x, x, \nu) \in M \times M \times]0, 1] \text{ for } x \in M, & \nu > 0, \\ (x, 0) \mapsto x \in M \subset TM \text{ as the zero section} & \text{for } \nu = 0. \end{cases} \tag{1}$$

- The range and source maps are defined as

$$\begin{cases} r(x, y, \nu) = (x, \nu) & \text{for } x \in M, \nu > 0, \\ r(z, X_z) = (z, 0) & \text{for } z \in M, X_z \in T_z M, \end{cases} \tag{2}$$

$$\begin{cases} s(x, y, \nu) = (y, \nu) & \text{for } y \in M, \nu > 0, \\ s(z, X_z) = (z, 0) & \text{for } z \in M, X_z \in T_z M. \end{cases} \tag{3}$$

- And finally the composition map is defined as

$$\begin{cases} (x, y, \nu) \cdot (y, z, \nu) = (x, z, \nu) & \text{for } \nu > 0 \text{ and } x, y, z \in M, \\ (z, X_z) \cdot (z, Y_z) = (z, X_z + Y_z) & \text{for } z \in M \text{ and } X_z, Y_z \in T_z M. \end{cases} \tag{4}$$

The topological structure. It is not difficult to understand that our tangent groupoid is, in fact, the disjoint union of two smooth ones ($G_1 = M \times M \times]0, 1]$ and $G_2 = TM$). We can endow this union with a suitable topology in order to obtain G_2 as the boundary of the whole set G, and G_1 as an open subset of G. This topology is given by specifying the convergence of sequences. Every convergent sequence on G_1 or G_2 will converge in our joined space. In addition, a sequence of elements of $\{(x_n, y_n, \nu_n) \mid (x_n, y_n, \nu_n) \in G_1\}$ converges to an element of the tangent bundle (z, X_z) if and only if, on any local chart, it satisfies

$$x_n^\mu \to z^\mu, \qquad y_n^\mu \to z^\mu, \qquad \frac{x_n^\mu - y_n^\mu}{\nu_n} \to X_z^\mu. \tag{5}$$

It is quite easy to prove the following:

Proposition 1. *The condition above does not depend on the choice of the local chart.*

Proof. Let us suppose two different charts U_i and U_j with non-vanishing overlapping, and the sequence $\{x_n, y_n, \nu_n\}$ of points in $M \times M \times]0, 1[$. The transition function will be Ψ_{ij} and we can write $\Psi_{ij}(y_n^\mu) = \Psi_{ij}(x_n^\mu + \nu_n X_{x_n}^\mu + \mathrm{o}(\nu^2)) = \Psi_{ij}(x_m^\mu) + \nu_n(\Psi_{ij})_*(X_{x_n}^\mu) + o(\nu^2)$ and thus $(y_n^\mu - x_n^\mu)/\nu_n = (\Psi_{ij})_*(X_{x_n}^\mu)$. This proves the result. □

It is also possible to prove that the tangent groupoid can be endowed with a differentiable structure:

Lemma 5. *The tangent groupoid is a smooth groupoid.*

The proof is quite technical, hence we refer the interested reader to [18, 19].

Let us consider now the case of $M = \mathbb{F}_N^n$, where N is the precision of the floating-point representation, and study the definition of discrete spaces inside it. It is trivial to see that $M \subset \mathbb{R}^n$, and therefore we can consider the points in M as corresponding to points in $\mathbb{R}^n$. Consider now the tangent groupoid of $\mathbb{R}^n$ and the definition of the topological structure above. As we know the topological structure, we can consider sequences of elements $(x_n, y_n, \nu_n) \in \mathbb{F}_N^n \times \mathbb{F}_N^n \times [0, 1]$, where $\nu_n = N^{-1}$ and study the elements of the tangent bundle obtained as limits. From the results above, it is obvious that the limit must be a vector X_p defined at the point $z \in \lim_{N\to\infty} \mathbb{F}^n = \mathbb{R}^n$, which is the limit of the sequences $\{x_n\}$ and $\{y_n\}$. If we define a smooth dynamical system on $\mathbb{R}^n$, this construction allows us to think in a sequence of discrete models defined on each $\mathbb{F}_N^n$ converging to that model; the higher the value of N, the higher the accuracy of the representation. As the dynamical system at the smooth level is defined by the flow of a vector field, we just need its discrete equivalent to define a discrete dynamical system. If we are able to define the analogues of all the geometric objects at the smooth level, we will be able to formulate the same structure for each value of N.

But of course, the main piece is the concept of vector field. Therefore, we define:

Definition 5. *A* discrete vector *at the point $p \in \mathbb{F}^n$ is a pair (p, q) where $q \in \mathbb{F}^n$. We will denote by $T_p\mathbb{F}^n$ the set defined as the union of all possible vectors defined at the point p, i.e.*

$$T_p\mathbb{F}^n = \{(p, q) \in \mathbb{F}^n \times \mathbb{F}^n\} \sim \mathbb{F}^n.$$

$T_p\mathbb{F}^n$ is called the tangent space at p. A simple example of a discrete vector can be given as follows. Let $c : [0, T] \to \mathbb{F}^n$ be a discrete curve on $\mathbb{F}^n$, with $c(0) = p$ and $[0, T] \subset \mathbb{F}$. We define a tangent vector $\Delta c(t)/\Delta t$ at $c(t)$ as follows:

$$\frac{\Delta}{\Delta t}c(t) = \frac{c(t + \delta) - c(t)}{\delta}, \tag{6}$$

where $\delta \in \mathbb{F}$, in section 4 we characterize this δ. In other words, the tangent vector at $c(t)$ is defined by two points $(c(t), c(t + \delta))$. There are various representations of vectors in the discrete setting. We shall encounter such definitions in section 4 where we also present, in detail, the algebraic and geometric properties of discrete vectors. For now we shall use the definition of vectors as given above.

We can consider the effect of discrete mappings at the level of vectors:

Lemma 6. *Let A and B be $\mathbb{F}^n$ spaces and $\Psi : A \to B$ be a discrete mapping. Then, the mapping $\Psi_{p*} : T_pA \to T_{\Psi(p)}B$, defined as $\Psi_{p*}(p, q) = (\Psi(p), \Psi(q))$, defines a one-to-one correspondence of the tangent spaces at the point $p \in A$ and $\Psi(p) \in B$.*

We demand for Ψ_{p*} to be discrete differentiable; see section 4.2. Again, at any point of the lattice, we can consider as many discrete vectors as points, i.e. the cardinality of the space of discrete vectors is 2^N.

We can take linear combinations of elements of $T_p\mathbb{F}^n$ with coefficients in $\mathbb{F}$, and then we can claim that an arbitrary linear combination of the form

$$\lambda_1 v_1 + \lambda_2 v_2 + \cdots + \lambda_k v_k \equiv (p, \lambda_1 q_1 + \cdots + \lambda_k q_k), \quad \lambda_i \in \mathbb{F}, \quad v_i \in T_p\mathbb{F}^n,$$

belongs to $T_p\mathbb{F}^n$. And now, this structure can be taken, in the continuum limit, to the usual vector space structure of $\mathbb{R}^n$, since the elements λ_i belong to $\mathbb{F}_N$, and this set goes to $\mathbb{R}$ in the limit. If we consider the canonical basis of $\mathbb{F}^n$, we see that each element $v \in T_p\mathbb{F}^n$ has, as coordinates,

$$v = v_1(1, 0, \ldots, 0) + \cdots + v_n(0, \ldots, 0, 1)$$

if $v = (v_1, \ldots, v_n) \in \mathbb{F}^n$. Summarizing, *any system of coordinates used to parametrize the points of* $\mathbb{F}$ *do define a coordinate system for the tangent space*. Another equivalent way of defining the coordinate system for the tangent space is explained, using the concept of discrete differentiability, in proposition 2.

When representing vectors, we will denote the canonical basis as

$$(0, \ldots, 0, \overbrace{1}^{i}, 0, \ldots, 0) \equiv v_i.$$

Remark 1. There are certain fundamental limitations in using the usual regular lattice approach towards a discrete mechanics. We present now a highly condensed summary of one particular problem (among many). The regular lattices can be defined in the same way as we have defined tangent spaces on nonregular spaces in definition 5. It is clear then that, in principle, an arbitrary combination of discrete vectors at a point p on the regular lattice with integer coefficients makes sense and it is closed in the tangent space denoted by $T_p\mathcal{R}^n_\epsilon$, where $\mathcal{R}^n_\epsilon$ denotes the regular lattice, i.e.

$$\lambda_1 v_1 + \lambda_2 v_2 + \cdots + \lambda_k v_k \equiv (p, \lambda_1 q_1 + \cdots + \lambda_k q_k), \quad \lambda_i \in \mathbb{Z}, \quad v_i \in T_p\mathcal{R}^n_\epsilon,$$

belongs to $T_p\mathcal{R}^n_\epsilon$, as long as the combination $\lambda_1 q_1 + \cdots + \lambda_k q_k$ belongs to $\mathcal{R}^n_\epsilon$. The problem of this construction is that it does not define a proper continuum limit, since even though in the limit it does provide linear combinations of real vectors, but it does so only with integer coefficients, since the scalars λ_i must belong to $\mathbb{Z}$ for the combination above to be closed. So we end up with the conclusion that the discrete structure defined on regular lattices does not go to the corresponding smooth structure on $\mathbb{R}^n$ in the continuum limit.

3.1.3. Discrete covectors

Definition 6. *Consider the discrete space* $\mathbb{F}^n$. A discrete covector α *at the point* $p \in \mathbb{F}^n$ *is defined as a mapping from any pair of points (i.e. a discrete vector) of the form* (p, q)*, where* $q \in \mathbb{F}^n$ *to* $\mathbb{F}$*. It can be represented as the link connecting* p *and* q *with the value of the function associated to the link. Since we can take a collection of vectors at a particular point, dual to this, we take the collection of discrete covectors and this collection is denoted by* $T^*_p\mathbb{F}^n$*, which is also called the cotangent space at* p*.*

Now we can study the analogue of the usual duality for real numbers. We can use the linear structure we defined for the vectors to define again the analogue of the duality product of the real case. Hence, we claim that the action of a vector $v_p \in T_p\mathbb{F}^n$ on a covector $\alpha_p \in T^*_p\mathbb{F}^n$ gives as a result a $\mathbb{F}$ number which is associated to the point p, i.e. we define a function. And now, unlike for a regular lattice case, this function is a $\mathbb{F}$-valued function and, hence, goes to

the limit to define the proper $\mathbb{R}^n$ function associated to the action of the smooth vector on the smooth covector.

There are no problems to considering duality in a natural way. We can consider the representation of covectors associated to the canonical basis of $\mathbb{F}^n$ that we used to represent vectors. We can then represent an element $\alpha_p \in T_p^*\mathbb{F}^n$ by the coordinates of the point $q \in \mathbb{F}^n$ and the link associated to the pair (p, q). We define thus a basis for the cotangent space $T_p^*\mathbb{F}^n$ as the set of elements Δx^i which are dual to the elements of the natural basis of $T_p\mathbb{F}^n$, i.e.

$$\langle \Delta x^i, v_j \rangle = \delta_i^j,$$

where δ_i^j is the Kronecker delta. Then, we can represent the elements of the cotangent space as all the linear combinations of these elements with coefficients in $\mathbb{F}$, i.e. any $\alpha_p \in T_p^*\mathbb{F}^n$ can be written as

$$\alpha_p = \sum_i \alpha_p^i \Delta x^i, \quad \alpha_p^i \in \mathbb{F},$$

where the set of floating-point numbers α_p^i locate the point $q \in \mathbb{F}^n$ which together with p defines the covector α_p and they also encode the value associated to the action on the vector (p, q).

In this context, we can study the duality product of vectors and covectors in terms of coordinates. Hence, given a vector $X_p \in T_p\mathbb{F}^n$ and a covector $\alpha_p \in T_p^*\mathbb{F}^n$, the duality product takes the form $\langle \alpha_p, X_p \rangle \in A(\mathbb{F}^n)$. We want to define this operation to be linear with respect to the additive structure, which we defined on the tangent and cotangent spaces. With the choice above, we can write, for any $\alpha_p = \sum_i \alpha_p^i \Delta^i \in T_p^*\mathbb{F}^n$ and $X_p = \sum_i X_p^i v^i \in T_p\mathbb{F}^n$,

$$\langle \alpha_p, X_p \rangle = \sum_{i=1}^{n} \alpha_p^i X_p^i \in \mathbb{F}.$$

Obviously, in the continuum limit we recover the usual vector–covector action.

3.1.4. Tensors. We now have vectors and covectors, so the definition of general tensors is completely straightforward:

Definition 7. *We shall call* discrete tensor contravariant of order *r and* covariant of order *s the elements* t_s^r *of the space*

$$(\mathcal{T}_p)_s^r = \{t \in T_p\mathbb{F}^n \times \cdots {}_{(r \text{ times})} \cdots \times T_p\mathbb{F}^n \times T_p^*\mathbb{F}^n \times \cdots {}_{(s \text{ times})} \cdots \times T_p^*\mathbb{F}^n\}.$$

As in the smooth case, completely symmetric and completely skew-symmetric tensors will be important, particularly the last (because we need k forms and multivectors to represent our mechanical objects).

3.2. Global objects

Definition 8. *We shall call* discrete tensor field contravariant of order *r and* covariant of order *s the mapping which assigns to each point of the discrete space* $\mathbb{F}^n$ a *discrete tensor of order r and covariant of order s:*

$$\mathcal{T} : \mathbb{F}^n \to (\mathcal{T}_p)_s^r.$$

The particular case of vector fields is then defined as:

Definition 9. *We shall call* discrete vector field *the mapping X which assigns to each point $p \in \mathbb{F}^n$ a discrete vector*

$$X(p) \in T_p\mathbb{F}^n \quad \forall p \in \mathbb{F}^n \Rightarrow X(p) = (p, q), \quad q \in \mathbb{F}^n.$$

From the representation we choose for the vectors, it is quite obvious that we can define the analogue of the flow of vector fields in a very straightforward manner:

Definition 10. *Let X be a discrete vector field. We shall call the* flow *of X the sequence of points in $\mathbb{F}^n$*

$$p_0, p_1, p_2, \ldots$$

such that

$$X(p_i) = (p_i, p_{i+1}).$$

It is also possible to extend the additive structure that we defined on $T_p\mathbb{F}^n$ to the space of discrete vector fields in the natural way: given two discrete vector fields X, Y, their sum $X + Y$ is defined as the vector field whose value at the point $p \in \mathbb{F}^n$ is given by the vector $X(p) + Y(p) \in T_p\mathbb{F}^n$.

Definition 11. *We shall call a* discrete k form *any mapping α which at every point $p \in \mathbb{F}^n$ assigns to the oriented hypersurface, defined by k-multivectors at that point p, a $\mathbb{F}$ value. We will represent that object as $\alpha(p \to p_1 \to \cdots \to p_n)$.*

We will denote by $\bigwedge^k(\mathbb{F}^n)$ the set of discrete k forms of the discrete space $\mathbb{F}^n$.

This definition allows us to consider functions trivially as 0 forms, since according to the definition it defines a hypersurface of dimension 0 (i.e. one point).

Then we define the wedge product:

Definition 12. *Let $\alpha \in \bigwedge^j(\mathbb{F}^n)$ and $\beta \in \bigwedge^k(\mathbb{F}^n)$. Then, we define the product $\alpha \wedge \beta$ to be the $(j + k)$-discrete form which assigns, at each point, of the discrete space, the hypersurface defined by the union of the $j+1$ points which define the j-dimensional hypersurface associated to α and the $k + 1$ points which define the k-dimensional hypersurface associated to β. If the union of the points does not define a hypersurface of dimension $j + k$ the wedge product is zero.*

The discrete exterior differential is a mapping $\Delta : \bigwedge^k(\mathbb{F}^n) \to \bigwedge^{k+1}(\mathbb{F}^n)$, defined in the following way. Consider, for instance, a function $f \in A(\mathbb{F}^n)$. The function corresponds to the assignment of an element of $\mathbb{F}$ at each point of the discrete space. The definition of a discrete one form implies that we must construct a covector at each point. We can do that in many different ways, but if we want to preserve at the discrete level the smooth property:

$$X(f) = \langle X, \Delta f \rangle,$$

the definition of the exterior differential must take into account the type of action that vector fields have on functions. For the forward difference method, this leads us to a definition of the exterior differential such as to define the one-form $\Delta f \in \bigwedge^1(\mathbb{F}^n)$ which for every point $p \in \mathbb{F}^n$ assigns to the one-dimensional hypersurface (i.e. a link) connecting each pair of points

(p, q), where the pair of points are defining a discrete vector, the value $f(q) - f(p)$. Hence, in the natural basis, we would obtain as a representation:

$$\Delta f(p) = \sum_i (f(p + h\epsilon_i) - f(p))\, \mathrm{d}x^i,$$

where h is the smallest possible distance from the point p to the next floating-point number in the ith direction of the point p, and $\epsilon_i = [0, \ldots, 1, 0, \ldots]^{\mathrm{T}}$. Analogously, given a one-form $\alpha \in \bigwedge^1(\mathbb{F}^n)$, we define the two-form $\Delta\alpha$ to be the mapping which for every point $p \in \mathbb{F}^n$ assigns to the surface, defined by a triplet of points (p, q, r) (where $q, r \in \mathbb{F}^n$), the value

$$\Delta\alpha(p \to q \to r) = \alpha(p \to q) + \alpha(q \to r) + \alpha(r \to p).$$

Lemma 7. *From the definition above, Δ is nilpotent:*

$$\Delta^2 = 0.$$

Proof. It is completely analogous to the usual proof of the boundary operator of simplicial homology being nilpotent. For instance, in the case of functions we have, for any $p, q, r \in \mathbb{F}^n$,

$$\begin{aligned}\Delta^2 f(p \to q \to r) &= \Delta f(p \to q) + \Delta f(q \to r) + \Delta f(r \to p) \\ &= f(q) - f(p) + f(r) - f(q) + f(p) - f(r) = 0.\end{aligned}$$ □

4. Representations of discrete vectors

We have seen that a tangent vector at a point $p \in \mathbb{F}^n$ is defined by a pair of points (p, q). In this section we give a few *representations* of tangent vectors. Let $A(\mathbb{F}^n)$ be the algebra of discrete functions on $\mathbb{F}^n$. The functions in $A(\mathbb{F}^n)$ are considered to be $\mathbb{F}$-valued functions. In the smooth setting, in order to define the concept of a tangent vector at a certain point, one considers functions defined in a neighbourhood (i.e. an open set) of that point. In the discrete setting however the concept of 'locality' is a bit different. We basically consider functions $f \in A_p(\mathbb{F}^n)$ defined on an open set around the point $p \in \mathbb{F}^n$. We have seen before that one particular way to explicitly define a discrete vector is as in (6). Then we have discrete vectors $v_i := (p, p + h\epsilon_i)$ defined as follows:

Definition 13 (The Euler discrete vector). *Define elements $v_1, \ldots, v_n \in T_p\mathbb{F}^n$ by letting*

$$v_i(f(p)) = \frac{f(p + h\epsilon_i) - f(p)}{h}, \tag{7}$$

where $\epsilon_i = [0, \ldots, 1, 0, \ldots]^{\mathrm{T}}$, and where h is the smallest possible distance from the point p to the next floating-point number[5] *in the ith direction of the point p. v_i is called a discrete vector and it has the following very important property:*

A Euler discrete vector at a point p is a linear map $v_i : A_p(\mathbb{F}^n) \to \mathbb{F}$ which satisfies the modified Leibniz rule:

$$v_i(f \cdot g) = v_i(f) \cdot g(p) + \mathrm{Aut}_{v_i}(f(p)) \cdot v_i(g), \quad \forall f, g \in A_p(\mathbb{F}^n), \tag{8}$$

[5] Note that the set of floating-point numbers is not a regular set, in the sense that the spacing between points changes in different regions. So the density of the points is different in different regions.

where Aut_{v_i} *is an automorphism which is a linear map* $\mathrm{Aut}_{v_i} : A_p(\mathbb{F}^n) \to \mathbb{F}$*, corresponding to the discrete vector* v_i*, defined as*

$$\mathrm{Aut}_{v_i}(f(p)) := f(p + h\epsilon_i), \quad p \in \mathbb{F}^n \tag{9}$$

such that $\mathrm{Aut}_{v_i}(f \cdot g) = \mathrm{Aut}_{v_i}(f) \cdot \mathrm{Aut}_{v_i}(g)\ \forall f, g \in A_p(\mathbb{F}^n)$.

Let us now see (8) by an example: consider two discrete functions $f, g \in A_p(\mathbb{F}^n)$. Then

$$\begin{aligned} v(f \cdot g) &= \frac{f(p + h\epsilon_i) \cdot g(p + h\epsilon_i) - f(p) \cdot g(p)}{h} \\ &= v(f(p)) \cdot g(p) + f(p + h\epsilon_i) \cdot v(g(p)) \\ &= v(f) \cdot g + \mathrm{Aut}_{v(f)}(f) \cdot v(g). \end{aligned}$$

In fact, *every* discrete vector, later on in this section we encounter other discrete vectors, has the fundamental property (8). An arbitrary Euler discrete vector $v := (p, p+\bar{\epsilon})$ in $T_p\mathbb{F}^n$ (where $\bar{\epsilon} = h \sum_i \lambda_i \epsilon_i$ and $\lambda_i \in \mathbb{F}$) is written as

$$v(f(p)) = \frac{f(p + \bar{\epsilon}) - f(p)}{h}$$

s.t. the modified Leibniz rule is satisfied, where $\mathrm{Aut}_v(f(p)) = f(p + \bar{\epsilon})$.

To summarize, we have that a Euler discrete vector $v : A_p(\mathbb{F}^n) \to \mathbb{F}$ is a linear mapping satisfying a modified Leibniz rule (8). From an algebraic geometric viewpoint such an object would be defined by the action of a *twisted derivation* (cf [10]), at a point p. We define on our discrete regular space $\mathbb{F}^n$:

Definition 14 (Discrete vector field)*. A discrete vector field is a linear mapping* $X : A(\mathbb{F}^n) \to A(\mathbb{F}^n)$ *which assigns to every point* $p \in \mathbb{F}^n$*, a Euler discrete vector* v_p *of* $T_p\mathbb{F}^n$ *as follows:*

$$X_p(f) := v(f(p))$$

and is a twisted derivation, i.e. it satisfies the following property; $X : A(\mathbb{F}^n) \to A(\mathbb{F}^n)$ *s.t.* $\forall f, g \in A(\mathbb{F}^n)$

$$X(f \cdot g) = X(f) \cdot g + \mathrm{Aut}_X(f) \cdot X(g),$$

where $\mathrm{Aut}_X : A(\mathbb{F}^n) \to A(\mathbb{F}^n)$ *s.t.*

$$\mathrm{Aut}_{X_p}(f(p)) = f(p + h\epsilon_i), \quad \forall p \in \mathbb{F}^n$$

and $(p, p + \bar{\epsilon})$*, of course, corresponds to discrete vectors at every point* $p \in \mathbb{F}^n$.

In the smooth setting there is a *unique* definition of vectors. Due to the lack of a limiting process, it turns out that (7) is just *one particular representation* of the smooth vector. Or from a discrete mechanics viewpoint, it is only a single element of a class of discrete vectors. Equation (7) is called the Euler discrete vector because it represents both the forward and the backward difference methods; the backward difference is expressed differently, i.e. as $(f(p) - f(p - h\epsilon_i))/h$ where f, p and ϵ_i are as defined in (7), but it has a similar structure as for (7). Similarly (7) can be rewritten to represent a central difference method, i.e. $(f(p + h\epsilon_i) - f(p - h\epsilon_i))(2h)$. One of main strengths of numerical analyses has been the large number of integration techniques available, for example, Euler techniques, Runge–Kutta, Verlet, Leapfrog among others. Each of these techniques is used heavily in practice, and there is a large amount of theoretical studies also done [20].

A fundamental question arises here—to what type of geometrical/mathematical entity in our framework do these various integration techniques correspond to? We start off by investigating the second-order Runge–Kutta method. We denote a second-order Runge–Kutta discrete vector by *rk*2. Below we are going to do roughly the following: given a discrete curve $y : [0, T] \to \mathbb{F}^n$, $[0, T] \subset \mathbb{F}$ we want to define a *rk*2 discrete vector at the point $y(t)$: first we use the Euler method to compute $y(t+\delta)$. Using this we *recompute* $y(t+\delta)$ by finding a point halfway across the time interval and using a midpoint discrete vector (to be made clear below) across the full width of the interval. Formally, we proceed as follows; let $\Delta y(t)/\Delta t$ be a Euler discrete vector, then first we compute $y(t+\delta)$ as follows:

$$\frac{\Delta y(t)}{\Delta t} =: f(y,t),$$

$$\Rightarrow y(t+\delta) = y(t) + \delta \cdot f(y,t).$$

Let $k_1 = \delta \cdot f(y,t)$. Then we recompute $y(t+\delta)$ as

$$y_{rk2}(t+\delta) = y(t) + \delta \cdot f(y(t) + k_1/2, t + \delta/2).$$

So now we have a new value for y at $t+\delta$ which we denote by $y_{rk2}(t+\delta)$. Then we have a new kind of discrete vector $\Delta/\Delta t|_{rk2}$:

$$\left.\frac{\Delta y(t)}{\Delta t}\right|_{rk2} = \frac{y_{rk2}(t+\delta) - y(t)}{\delta}$$

which we call the *rk*2 discrete vector. Note that the *rk*2 discrete vector can also be called a midpoint discrete vector (since it is nothing more than a midpoint derivative!). We can extend the above idea to Runge–Kutta methods of *any order*, see [12] for more details. Now consider the *rk*2 discrete vector. A collection of such objects (when we consider an equivalence class of discrete curves, [12]) forms a free module structure (like we have seen before for the Euler discrete vector). This is the tangent space formed by *rk*2 discrete vectors. This tangent space is different from the tangent space formed by Euler vectors. We use the usual notation $T_p\mathbb{F}^n$, it should be clear from the context what type of elements are used to define the tangent spaces. Now consider functions $f \in A_p(\mathbb{F}^n)$. Then we have

Definition 15 (Runge–Kutta vector). *Let* $k = \epsilon \cdot v_i(f(p))$ *from* (7). *Define elements* $v_1|_{rk2}, \ldots, v_n|_{rk2} \in T_p\mathbb{F}^n$ *by letting*

$$v_i|_{rk2}(f(p)) = \frac{f_{rk2}(p + h\epsilon_i) - f(p)}{h}, \tag{10}$$

where

$$f_{rk2}(p + h\epsilon_i) = f(p) + h\epsilon_i \cdot v_i(f(p) + k/2).$$

$v_i|_{rk2}$ *is called a rk*2 *discrete vector and it satisfies the modified Leibniz rule, i.e.*

$$v_i|_{rk2}(f \cdot g) = v_i|_{rk2}(f) \cdot g + \mathrm{Aut}_{v_i|_{rk2}}(f(p)) \cdot v_i|_{rk2}(g) \quad \forall f, g \in A_p.$$

A similar definition can be written for Runge–Kutta vectors of any order. Hence a Runge–Kutta vector is also a discrete vector. Furthermore, one can easily show that the Leapfrog method can also be incorporated into our setting, thereby giving us a Leapfrog discrete vector. *Hence one can see how a wide variety of integration techniques turn out simply to be nothing more than just discrete vectors in our setting.*

Finally, we introduce another type of discrete vector in the discrete setting. This basically arises when discrete curves $q(t)$ and $\phi(t)$ are given on $\mathbb{F}^n$, and we have a set of difference equations of the type

$$v(q(t)) = \phi(t), \qquad v(\phi(t)) = q(t)$$

and instead of using a Euler discrete vector v we wish to use the second-order Runge–Kutta technique. In that case we would end up with the following set of equations:

$$\bar{q}(t) = q(t) + \delta\frac{\phi(t)}{2}, \qquad \bar{\phi}(t) = \phi(t) + \delta\frac{q(t)}{2},$$
$$q(t+\delta) = q(t) + \delta\bar{\phi}(t), \qquad \phi(t+\delta) = \phi(t) - \delta\bar{q}(t).$$

On further manipulation of the above equations we obtain expressions for $v(q(t))$ and $v(\phi(t))$:

$$\frac{q(t+\delta) - q(t)\cdot c}{\delta} = \phi(t) = v(q(t)), \qquad \frac{\phi(t+\delta) - \phi(t)\cdot \bar{c}}{\delta} = q(t) = v(\phi(t)),$$

where $c = 1 - \delta^2/2$ and $\bar{c} = \delta^2/2 - 1$. Now let us see how v acts on any pair of functions $f, g \in A(\mathbb{F}^n)$:

$$\begin{aligned} v(f\cdot g) &= \frac{f(t+\delta)g(t+\delta) - f(t)g(t)\cdot c}{\delta} \\ &= \frac{f(t+\delta)g(t+\delta) - f(t+\delta)g(t) + f(t+\delta)g(t) - f(t)g(t)\cdot c}{\delta} \\ &= \frac{f(t+\delta) - f(t)\cdot c}{\delta}g(t) + f(t+\delta)\frac{g(t+\delta) - g(t)}{\delta}. \end{aligned}$$

In other words, the action of this new kind of vector on a pair of discrete functions results in a special kind of modified Leibniz rule wherein instead of having the same vector acting on both the functions, we have this vector action on f, but on the function g it is the Euler discrete vector that is acting. Hence we have:

Definition 16 (Mixed discrete vectors). *Let $f \in A_p(\mathbb{F}^n)$. Then $\tilde{v}$ is a mixed discrete vector at a point $p \in \mathbb{F}^n$, i.e. it is a linear mapping $\tilde{v} : A_p(\mathbb{F}^n) \to \mathbb{F}$ defined as*

$$\tilde{v}(f(p)) = \frac{f(p + h\epsilon_i) - f(p)\cdot c}{h}; \qquad c = 1 - \frac{h^2}{2}$$

and s.t. it satisfies the mixed-modified Leibniz rule

$$\tilde{v}(f\cdot g) = \tilde{v}(f)\cdot g(p) + \mathrm{Aut}_{\tilde{v}(f)}(f(p))\cdot v(g),$$

where v is the ordinary discrete vector defined in (7) *and* Aut *is as defined in* (9).

There is of course yet another mixed discrete vector above, corresponding to $c = h^2/2 - 1$. We do not classify the set of possible discrete vectors, we only conjecture that there may be many more discrete vectors! Corresponding to a mixed discrete vector, we have a mixed discrete vector field $\tilde{X}$, defined in the same way as a discrete vector field. So $\tilde{X} : A(\mathbb{F}^n) \to A(\mathbb{F}^n)$ s.t. at every point it defines a mixed discrete vector and it satisfies a mixed-modified Leibniz rule, hence *we have defined a new algebraic object—the mixed twisted derivation*. So the elements of our tangent spaces are (mixed) discrete vectors[6].

[6] Henceforth, we only say 'discrete vectors' to imply either ordinary discrete vectors or mixed discrete vectors, it will be clear from the context which discrete vectors we are using.

4.1 Action of vector fields on functions

4.1.1 Twisted derivations. Towards the end of section 3.2 we have discussed the type of action that vector fields must have on functions; this has important implications on the algebraic structures which can be defined on the set of functions $A(\mathbb{F}^n)$. From the study of the continuum limit (using the tangent groupoid construction) we know, formally, that the action of the vector fields on functions must be of the form

$$X(f)(p) = f(q) - f(p), \qquad X(p) = (p, q) \in T_p\mathbb{F}^n.$$

On the other hand, for the case of nonregular lattice $\mathbb{F}^n$, we can define an algebraic structure on the set of functions $A(\mathbb{F}^n)$ as a direct analogue of the pointwise algebraic structure of the smooth case. Hence we have:

Definition 17. *We can endow the set $A(\mathbb{F}^n)$ with a commutative algebraic structure by defining $(f \cdot g)(p) = f(p)g(p)$. As now the product in $\mathbb{F}$ is closed, the definition above is well defined and commutative.*

But this definition implies also that X does not define a derivation of this pointwise algebra of functions. It does define an alternative structure, and is a twisted derivation, as in definition 14.

This property has other implications, as for instance the fact that the action of the vector fields does not necessarily satisfy the chain rule. For instance, consider the action of a derivation on the function $f(x) = x^2$. From the definition of twisted derivation we have $X(f)(x) = X(x^2) = X(x) \cdot x + \mathrm{Aut}_X(x) \cdot X(x)$. Only if $\mathrm{Aut}_X(x) = x$ for any vector field X, the chain rule is satisfied.

Note that our tangent spaces are free $\mathbb{F}$-modules, which means that they have a set of linearly independent generators. We have already seen in section 3.1 how one can define such a set. Now we define this 'basis' set from another point of view, by using a concept of discrete differentiability. This concept will also help us to formalize the behaviour of discrete vectors under a coordinate transformation.

4.2 Discrete differentiability

The notion of a discrete differentiability is crucial. In the smooth setting the concept of differentiability is used to distinguish between various functions. Similarly, it is possible to do so in the discrete setting, and also our definition will, in the limit, correspond to the usual definition of differentiability in the smooth case. We first adapt the definition of the smooth case here:

Definition 18. *A function $f : \mathbb{F}^n \to \mathbb{F}$ is said to be* discrete-differentiable *at $p \in \mathbb{F}^n$ iff there exists a mapping $G : A(\mathbb{F}^n) \to \mathbb{F}^n$ s.t.*

$$\lim(d(p, p_1) \to h) \frac{f(p_1) - f(p) - G(f(p)) \cdot d(p - p_1)}{d(p, p_1)} = 0,$$

where $d(p, p_1)$ is the distance between the points read from the smooth metric and h is again the smallest distance achievable at the point p.

Remark 2. From the above definition it might seem that any, and every, discrete function on $\mathbb{F}^n$ is discrete-differentiable!, after all we are not demanding a continuum limiting process. The only things that we need are the values of f at the points $p + \epsilon_i$ and at p, so it seems that

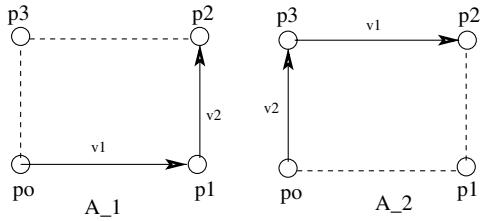

Figure 1. Path vectors of a two-dimensional function, $A_1 = v_2 \ominus v_1, A_2 = v_1 \ominus v_2$.

the definition is of no formal use. Fortunately, this is not the case in general. Indeed, since we are working with floating-point numbers it can very easily happen that $f(p + \epsilon_i) - f(p)$ gives a result which is an indeterminate element in $\mathbb{F}$ (very much like the ∞ element of the reals) called the overflow element [14]. This occurs when the result is too large to be definable in $\mathbb{F}$, so a special element is assigned to the result of such computations. In this case the above definition is not satisfied. A lot of such overflow, or underflow, situations can happen and, hence, there are many discrete functions that are not discrete differentiable! Moreover note that, in the continuum limit, we recover the usual definition of differentiability, and then $L \in \mathbb{F}$ (where L is the largest element in $\mathbb{F}$) would correspond to the ∞ element of the reals.

To formalize the above remark we need an extra notion—that of discrete 'smoothness'.

Definition 19 (Discrete smoothness). *A function $f : \mathbb{F}^n \to \mathbb{F}$ is said to be smooth, in a discrete sense, around a point $p \in \mathbb{F}^n$, if in an open set around the point p we have that*

$$|f(p + h\epsilon_i) - f(p)| < L,$$

where L is the largest number in $\mathbb{F}$.

We explain in detail the discrete differentiability of a two-dimensional function $g : \mathbb{F}^2 \to \mathbb{F}$. The one-dimensional case $f : \mathbb{F} \to \mathbb{F}$ is straightforward; define

$$G(f(p)) \cdot h\epsilon_i = v(f(p)) \cdot h\epsilon_i,$$

where $v(f)$ is as defined in (7). This satisfies the definition of discrete differentiability (by direct substitution) for one-dimensional functions $f : \mathbb{F} \to \mathbb{F}$.

For the two- (and higher)-dimensional case things are a little different because, as we will make clear soon, there is more than one *path* along which the discrete differentiability of the function can be defined. We want to know when $f : \mathbb{F}^2 \to \mathbb{F}$ is differentiable at a point $p \in \mathbb{F}^2$. At a point $p \in \mathbb{F}^2$ define the *path vectors* v_1 and v_2 (see figure 1) as

$$v_1(f(p)) = \frac{f(p + (h, 0)) - f(p)}{h}, \qquad v_2(f(p)) = \frac{f(p + (0, h)) - f(p)}{h}.$$

Note that in the above we have assumed that the point spacings are the same and, hence, we used a single ϵ to indicate the equal spacing. This result holds in the general case also, but notationally it is much simpler to assume equal point spacings. Then define the *concatenation* of these path vectors as follows:

$$(v_2 \ominus v_1)(f(p)) := \frac{f(p + (h, 0)) - f(p)}{h} + \frac{f(p + (h, h)) - f(p + (h, 0))}{h}. \tag{11}$$

However in the discrete case, since we do not have a limiting process as in the smooth case we obtain an *equivalence class of concatenations* depending on the path taken to define the

vectors (see figure 1). In the smooth case we do not have such a situation, because in the limit all points (that are an ϵ distance from p) converge to p, implying that in the limit there is no such thing as a path. *What the above equation implies is that any discrete vector v_p at a point p on $\mathbb{F}^2$ can be written as a concatenation of two path vectors, v_1 and v_2.*

Now we come to the differentiability of the two-dimensional function. Define

$$G(f) = \frac{f(p+(h,0)) - f(p)}{h} + \frac{f(p+(h,h)) - f(p+(h,0))}{\epsilon}$$
$$\Rightarrow G(f)\cdot\epsilon_i = f(p+(h,0)) - f(p) + f(p+(h,h)) - f(p+(h,0)).$$

With this choice for G, we have differentiability for the two-dimensional case, this can be checked by direct substitution of G into definition 18. Note that discrete differentiability is *independent* of the path taken, as can be easily seen when we substitute the above choices of G (i.e. $v_1 \ominus v_2$ or $v_2 \ominus v_1$) into the definition of discrete differentiability. G is called the gradient of the function and our definition of G is coordinate free. Extending this idea to higher-dimensional discrete vectors, an n-dimensional discrete vector v_p at the point p on $\mathbb{F}^n$, can be written as the concatenation of n path vectors, i.e.

$$v_p = c_1 v_1 \ominus c_2 v_2 \ominus \cdots \ominus c_n v_n \tag{12}$$

or any other $n!$-linear combination of the above elements. Hence we have an equivalence class, of representations, with $n!$ elements. Using this in the next section we will define the set of linear independent elements generating the tangent spaces on discrete manifolds.

5. Discrete manifolds

In the previous section we have defined a discrete calculus on $\mathbb{F}^n$. We have seen what discrete vectors and discrete covectors are and we have seen the concept of discrete differentiability. In this section we take a very brief look at the concept of discrete manifolds, and we would like to transfer the discrete calculus onto these manifolds. Discrete manifolds locally look like the space of floating-point numbers $\mathbb{F}^n$. Now we define a *topological structure* for $\mathbb{F}^n$. Firstly, $\mathbb{F}^n \subset \mathbb{R}^n$. The topology of $\mathbb{R}^n$ is given by balls of some radius centred on the points of $\mathbb{R}^n$. Then the topology of $\mathbb{F}^n$ is given by the intersections of the open sets of $\mathbb{R}^n$ (which are defining a topology for $\mathbb{R}^n$) with the open sets of $\mathbb{F}^n$. Those intersections which do not contain any points of $\mathbb{F}^n$, simply correspond to the empty set of $\mathbb{F}^n$. Also note that these balls may or may not be centred on the points of $\mathbb{F}^n$, and we only need that the balls contain the points of $\mathbb{F}^n$. It is easy to see that these sets of balls satisfy the axioms of topology and hence define a topology for $\mathbb{F}^n$. Thus we have a *relative topology* with respect to the Euclidean $\mathbb{R}^n$ topology.

Next we need a metric. We restrict the metric of $\mathbb{R}^n$ to $\mathbb{F}^n$. By this we mean that the distance between any two points in $\mathbb{F}^n$ is given by a floating-point number and where this floating point number is obtained by a finite-precision representation of the distance that is actually represented by a 'real' number. But what is the nature of the restricted metric when it is given by floating-point numbers? It is a *pseudo-metric*—so it fulfils the basic metric properties, i.e. it is nonnegative, symmetric and satisfies the triangular inequality. But it does not satisfy the condition $d(x, y) = 0 \Leftrightarrow x = y$. This happens because of the rounding-off truncation property of floating point numbers.

Now let $\mathcal{Z}$ be a discrete set which is also a topological manifold. Suppose that for any $l \in \mathcal{Z}$ there exists an open set U containing l, and a bijection ψ mapping U onto some open subset of $\mathbb{F}^n$ for some fixed n. $\mathbb{F}^n$ is a special kind of a *free module* over $\mathbb{F}$ of finite rank n; see [12, 21] for more details. Hence, we have on $\mathbb{F}^n$ the natural coordinate functions (i.e. basis

elements) denoted by r_i, $i := \{1, \ldots, n\}$. Then by composition with ψ we obtain coordinate functions z_i, $i := \{1, \ldots, n\}$ on U by letting $z_i = r_i \circ \psi$; (U, ψ) is called a coordinate chart. As we have seen in definition 18, there exists a notion of *discrete differentiability* on $\mathbb{F}^n$ and, of course, we would then like to transfer this notion onto $\mathcal{Z}$ also. In order to do this we impose the conditions that the coordinate chart mappings ψ be homeomorphisms and that the corresponding coordinate transformation maps $S = \psi \circ \phi^{-1} : \phi(U \cap V) \to \psi(U \cap V)$ be discrete-differentiable. The second condition is known as *compatibility of coordinate charts*. The collection of compatible coordinate charts is said to be an *atlas*, and we define that there exists a maximal atlas if any coordinate chart (U, θ), that is compatible with any coordinate chart of the atlas, also belongs to the atlas.

Definition 20. *Let $\mathcal{Z}$ be a discrete topological set*[7] *(so it automatically Hausdorff). Then $\mathcal{Z}$ is a discrete-differentiable manifold if it has a maximal atlas.*

Now we study an important property for discrete manifolds, the discrete differential of a mapping.

Definition 21 (Tangent map). *Let M, N be two discrete space of $\mathbb{F}^n$-type, and let $F : M \to N$ be a discrete-differentiable mapping between them. The discrete differential of the mapping F at the point $p \in M$, denoted by F_{*p}, is a linear mapping $F_{*p} : T_pM \to T_{F(p)}N$ and is defined as*

$$[F_{*p}(X_p)](f) = X_p(f \circ F), \quad \forall f \in A(N).$$

This mapping, which is discrete-differentiable, is called the tangent map.

We have introduced tangent spaces in section 3.1. Now we have all the necessary ingredients to define the basis of a tangent space. Note that since we are not dealing with vector spaces, it is not correct to use the terminology 'basis'—however for this paper we stick to this abuse of notation. Denote discrete vectors (either ordinary or mixed) in $T_p\mathbb{F}^n$ by v_{ip}. Then

$$v_{ip}(\bar{r}_j) = \delta^i_j, \quad i, j \in \{1, \ldots, n\},$$

where $\bar{r}_j$ are the coordinate functions on $\mathbb{F}^n$. Since $\bar{r}_j$ are independent natural coordinates on $\mathbb{F}^n$, it follows that $\{v_{1\,p}, \ldots, v_{n\,p}\}$ are independent module elements in $T_p\mathbb{F}^n$. The following proposition shows that these independent elements are actually the basis of the tangent space.

Proposition 2. $\{v_{1\,p}, \ldots, v_{n\,p}\}$ *form a basis of the tangent space $T_p\mathbb{F}^n$.*

Proof. We have seen that on $\mathbb{F}^n$, any discrete vector v_p is written as the concatenation of path vectors. So for an n-dimensional tangent space we can write v_p by a concatenation of n-path vectors as in (11). This directly implies that for any function $f \in A_p(\mathbb{F}^n)$, the action of an arbitrary discrete vector v_p on f can be written as

$$v_p(f) = c_1 v_1(f) \circ c_2 v_2(f) \circ \cdots \circ c_n v_n(f) = \sum_{i=1}^{n} c_i v_{ip}(f).$$

Hence $\{v_{1\,p}, \ldots, v_{n\,p}\}$ form a basis of the tangent space. □

[7] Since $\mathcal{Z}$ is a finite set, it is second countable.

Now we move onto discrete manifolds $\mathcal{Z}$. For any point $l \in \mathcal{Z}$ we associate a coordinate chart (U, Ψ), where U is a neighbourhood of the point l, and the map $\psi : U \subset \mathcal{Z} \to Y \subset \mathbb{F}^n$ is a homeomorphism. Now we define the *tangent map* between $\mathcal{Z}$ and $\mathbb{F}^n$. Let $T_l\mathcal{Z}$ be the tangent space of $\mathcal{Z}$ at the point l, and denote its elements by $\eth|_l$. Given $\psi : \mathcal{Z} \to \mathbb{F}^n$, the tangent map (at l) is a linear mapping $\psi_*|_l : T_l\mathcal{Z} \to T_{\psi(l)}\mathbb{F}^n$ defined as

$$[\psi_*|_l(\eth|_l)](f) = \eth|_l(f \circ \psi), \quad \forall f \in A_{\psi(l)}(\mathbb{F}^n). \tag{13}$$

Once this is done we then have a *basis for the tangent space* $T_l\mathcal{Z}$:

$$\eth_1|_l, \ldots, \eth_n|_l$$

by letting $\eth_i|_l := \psi_{*l}^{-1}(v_{i|_{\psi(l)}})$, since ψ is an homeomorphism we can do this. With this definition we have for any $g \in A(\mathcal{Z})$

$$\eth_i|_l(g) = \psi_{*l}^{-1}(v_{i|_{\psi(l)}})(g) = v_{i|_{\psi(l)}}(g \circ \psi^{-1}) = v_{i|_{\psi(l)}}(\hat{g}) = v_i(\hat{g})(z^1(l), \ldots, z^n(l)),$$

where $\hat{g} = g \circ \psi^{-1}$ is the local representation of g. If X_l is an arbitrary element of $T_l\mathcal{Z}$, then for any $g \in A_l(\mathcal{Z})$, we have the following expression for X_l: $X_l(g) = \sum_i c_i \eth_i|_l(g)$, for constants $c_i \in \mathbb{F}$. Hence $X_l(g)$ is just the (discrete version of the) directional derivative of the function g in the direction of the discrete vector $(c_1, \ldots, c_n)^{\mathrm{T}}$, at the point $l \in \mathcal{Z}$. Note that $(c_1, \ldots, c_n)^{\mathrm{T}}$ is the discrete vector representation of X_l in the basis $(\eth_1|_l, \ldots, \eth_n|_l)$.

We demand that the coordinate transformation maps be related in a discrete differentiable manner, i.e. given two coordinate charts $(\psi, U), (\Phi, V)$ at a point $l \in \mathcal{Z}$ on a discrete manifold $\mathcal{Z}$, and a coordinate transformation map $S = \psi \circ \Phi^{-1}$; a discrete vector $\eth|_l \in T_l\mathcal{Z}$ can be written w.r.t. the two charts as $\eth|_l = \sum \alpha_i \eth x_i$ for the chart (Φ, U), or $\eth|_l = \sum \beta_j \eth z_j$ for the chart (ψ, V). Then the coefficients α_i and β_i are related as (summation over the indices is assumed) $\beta = \eth_x S(x(l))\alpha$. This is what we meant by demanding compatible coordinate charts for an atlas, i.e. the map $S = \psi \circ \Phi^{-1} : \Phi(U \cap V) \to \psi(U \cap V)$ be an C^m-isomorphism.

The analogous concept of a *vector field* on configuration space is a discrete vector field which we already encountered in definition 14. Now we define a discrete vector field on a discrete manifold.

Definition 22. *We shall call* discrete vector field *the mapping X which assigns to each point $l \in \mathcal{Z}$ a discrete vector*

$$X(l) \in T_l\mathcal{Z}, \quad \forall l \in \mathcal{Z} \Rightarrow X(l) = (l, m), \quad l \in \mathcal{Z}.$$

From the representation we choose for the vectors, it is quite obvious that we can define the analogue of the flow of vector fields in a very straightforward manner:

Definition 23. *Let X be a discrete vector field. We shall call the* flow *of X the sequence of points in $\mathcal{Z}$*

$$l_0, l_1, l_2, \ldots$$

such that

$$X(l_i) = (l_i, l_{i+1}).$$

It is also possible to extend the additive structure that we defined on $T_p\mathbb{F}$ to the space of discrete vector fields in the natural way: given two discrete vector fields X, Y, their sum

$X + Y$ is defined as the vector field whose value at the point $l \in \mathcal{Z}$ is given by the vector $X(l) + Y(l) \in T_l\mathcal{Z}$.

5.1. Cotangent spaces

We have defined discrete covectors on $\mathbb{F}^n$ in definition 6. We now define this on the discrete manifold. Since the tangent space $T_l\mathcal{Z}$ is a free module, there exists a dual free module, of the same dimension, defined as:

Definition 24. *Let ∂_{z_i} be the basis of the tangent space $T_l\mathcal{Z}$, corresponding to the coordinate functions z_i of the algebra A. Then we denote the set of basis elements of the dual free-module $T_l^*\mathcal{Z}$, called the cotangent space, by $\{\Delta z_i|_l\}$ such that*

$$\Delta z^i|_l(\partial_{z_j}|_l) = \delta^i_j.$$

Since the tangent space is a free module, hence the cotangent space is also a free module and so any discrete covector can be written as $\sum_{i=1}^n \alpha_i \Delta z_i|_l$. Given two overlapping coordinate charts (U, z_i) and (V, x_i) around $l \in \mathcal{Z}$, any discrete covector $\sigma_l \in T_l^*\mathcal{Z}$ can be expressed by, summing over the indices, $\sigma_l = \alpha_i \Delta z_i|_l$ or $\sigma_l = \beta_j \Delta x_j|_l$. Then the coefficients α_i and β_i are related as $\alpha = \beta \partial S/\partial x(x(l))$ (summation is assumed).

Just as discrete vector fields are the global objects corresponding to discrete vectors, discrete one-forms are the global objects corresponding to discrete covectors. Loosely speaking, a one-form is a map that assigns to each point $l \in \mathcal{Z}$ a discrete covector at that point. Proceeding along such lines we can define tangent/cotangent bundles and their associated structure; see [12] for further details.

6. Discrete Hamiltonian mechanics

In the following subsection we give a brief description of how we represent system dynamics in our discrete setting. Then we restrict ourselves to Hamiltonian dynamics.

6.1. Discrete dynamics

We want to introduce dynamics in the geometrical framework described above. Let us consider then a discrete manifold $\mathcal{Z}$, with the corresponding algebra of functions $A(\mathcal{Z})$. A trajectory on $\mathcal{Z}$ will be a sequence of points in the form $\{x_i\}_{i\in\mathbb{F}}$ (which can alternatively be seen as a sequence of elements of the algebra of discrete functions). We can represent them, if we consider for instance the trajectory from an initial point at time $t = 0$ and a final point at time $t = T$ as a point in $\mathcal{Z}_0 \times \cdots \times \mathcal{Z}_T$, where x_i belongs to the ith copy of $\mathcal{Z}$. From a practical point of view, very often we will not be obtaining the positions for all possible values of time, but just for a subset. If we consider a constant time step δ, the trajectory will be of form $(x_o, x_\delta, x_{2\delta}, \ldots)$.

Note that if the discrete system is the result of a discretization of a continuous system, this corresponds to, roughly speaking, an *integrator*; see, for example, [2] and the references therein for details about various integrators and their properties. There are several ways to define the algorithm describing the system evolution. Baez and Gilliam [8] and Gilliam [9] have developed the algorithm for the Lagrangian framework in the context or ordinary derivations (i.e. those that satisfy the usual Leibniz rule). In this paper, we develop the algorithm for the Hamiltonian framework, and in the twisted derivation setting. There are two ways in which we can proceed from here—the symplectic approach or the Poisson approach. The symplectic approach faces an important technical problem: using two copies of the algebra it is clear that

we can represent velocity in this discrete setting. However it is not clear how to represent momenta in a canonical manner. Hence we are unable to develop Hamiltonian mechanics from this viewpoint.

6.2. Poisson manifolds

In the smooth case, the Poisson structure is usually defined in two ways. One is by the generalization of the symplectic structure, i.e. let (M, w) be a symplectic manifold, $f, g \in C^\infty(M)$ and $X_f, X_g \in \mathcal{X}(M)$ be the corresponding vector fields, then the Poisson bracket is the function $\{f, g\} = w(X_f, X_g)$. In our formulation, we are unable to do the above, as yet, since we do not know how to define a canonical symplectic form. Another way is to use a completely anti-symmetrical tensor field of order $(2, 0)$, whose action on a pair of exact one-forms defines a Poisson bracket. We proceed in this latter setting.

Definition 25 (The discrete Poisson bracket). *Let $\mathcal{Z}$ be a discrete manifold and consider the algebra of discrete differentiable functions $A(\mathcal{Z})$ on $\mathcal{Z}$. Consider a skew-symmetric $(2, 0)$ tensor $J : \Lambda^1(A) \times \Lambda^1(A) \to A(\mathcal{Z})$. J defines a Poisson bracket by its action on a pair of exact one-forms as follows:*

$$\{f, g\} := J(\Delta f, \Delta g) \tag{14}$$

such that $\{\cdot, \cdot\}$ is a skew-symmetric, bilinear operation on $A(\mathcal{Z})$, and $\{\cdot, \cdot\}$ defines discrete vector fields from function as follows:

$$\forall f \in A(\mathcal{Z}), \qquad f \mapsto X_f = \{f, \cdot\} = J(\Delta f, \cdot) \in \mathfrak{X}(\mathcal{Z}).$$

Moreover $\{\cdot, \cdot\}$ satisfies the following modified Leibniz rule, i.e. for functions $f, g, h \in A(\mathcal{Z})$,

$$\{f, g \cdot h\} = \{f, g\} \cdot h + \mathrm{Aut}_{X_f}(g) \cdot \{f, h\}.$$

J is called a discrete Poisson tensor. A discrete manifold $\mathcal{Z}$ whose algebra of functions $A(\mathcal{Z})$ is endowed with a Poisson bracket is called a discrete Poisson manifold.

Definition 26. *Let $\mathcal{Z}$ be a Poisson manifold and $H \in A(\mathcal{Z})$. The* Hamiltonian discrete vector field[8] *associated with H is the unique discrete vector field X_H satisfying $X_H(f) = \{f, H\} = -\{H, f\}$ for every $f \in A(\mathcal{Z})$.*

$\{,\}$ as defined above should actually be called *almost Poisson*, since we are not asking it to satisfy any kind of Jacobi identity. The reason is that, in a first analysis, it is a condition too restrictive. We can admit brackets which, not satisfying the Jacobi identity at the discrete level, recover it in the continuum limit. We refer the interested reader to [12] for further details.

Example 4. Consider the discrete space $\mathbb{F}^{2n}$ and the Poisson bracket defined by the following assignment:

$$\{f, \cdot\} = X_f = \eth_{z^i} f \eth_{z^{i+n}} - \eth_{z^{i+n}} f \eth_{z^i}.$$

[8] Discrete analogue of a Hamiltonian vector field.

Hence, the Poisson bracket becomes

$$\{f, g\} = X_f(g) = \eth_{z^i} f \eth_{z^{i+n}} g - \eth_{z^{i+n}} f \eth_{z^i} g.$$

Now let us check the properties of this simple bracket. Skew symmetry and bilinearity are obvious. The modified Leibniz rule is

$$\begin{aligned}\{f, g \cdot h\} &= \eth_{z^i} f \eth_{z^{i+n}} (g \cdot h) - \eth_{z^{i+n}} f \eth_{z^i} (g \cdot h) \\ &= \eth_{z^i} f \eth_{z^{i+n}} g \cdot h + \eth_{z^i} f \eth_{z^{i+n}} h \cdot \mathrm{Aut}_{(\eth_{z^{i+n}} g)}(g) \\ &\quad - [\eth_{z^{i+n}} f \eth_{z^i} g \cdot h + \eth_{z^{i+n}} f \eth_{z^i} h \cdot \mathrm{Aut}_{(\eth_{z^i} g)}(g)] \\ &= \{f, g\} \cdot h + \mathrm{Aut}_{(\eth_z f)}(g) \cdot \{f, h\}.\end{aligned}$$

A manifold $\mathcal{Z}$, where $A(\mathcal{Z})$ is equipped with a Poisson bracket, is called a *Poisson manifold*, the bracket defining a Poisson structure on $A(\mathcal{Z})$.

From a practical point of view, it is interesting to be able to present coordinate expressions of the bracket. In this paper, we will consider only the case of discrete spaces. The case for general discrete manifolds will be studied in a future paper. For the particular case of $\mathcal{Z} = \mathbb{F}^n$, we can consider the coordinate expressions with respect to the natural basis $\{z^i\}$. We can then write

$$\{f, g\} = \nabla f \cdot J \nabla g = \sum_{ij} \eth_{z^i} f J^{ij} \eth_{z^j} g, \tag{15}$$

where $\nabla(f) = (\eth_{z^i} f)$ is the gradient of the function f, and is a column of discrete vectors. The term $J_{ij}(z)$ represents a skew-symmetric matrix. In this situation, the discrete Hamiltonian vector field associated to a function $f \in A(\mathbb{F}^n)$ reads

$$X_f = \{f, \cdot\} = \sum_{ij} \eth_{z^i} f J^{ij} \eth_{z^j}.$$

In this case we can even study the Jacobi identity and, hence, the true analogue of smooth Poisson brackets. For instance, in the case of example 4, we can consider, given functions $f, g, h \in A(\mathbb{F}^n)$,

$$\begin{aligned}\{\{f, g\}, h\} + \{\{h, f\}, g\} + \{\{g, h\}, f\} &= \{\eth_q f, g\}[\eth_p h - \mathrm{Aut}(\eth_p h)] \\ &\quad - \{\eth_p f, g\}[\eth_q h - \mathrm{Aut}(\eth_q h)] + \{\eth_q g, h\}[\eth_p f - \mathrm{Aut}(\eth_p f)] \\ &\quad - \{\eth_p g, h\}[\eth_q f - \mathrm{Aut}(\eth_q f)] + \{\eth_q h, f\}[\eth_p g - \mathrm{Aut}(\eth_p g)] \\ &\quad - \{\eth_p h, f\}[\eth_q g - \mathrm{Aut}(\eth_q g)].\end{aligned} \tag{16}$$

Note that in the continuum limit we directly recover the classical Jacobi identity $\{\{f, g\}, h\} + \{\{h, f\}, g\} + \{\{g, h\}, f\} = 0$. This is easy to see; consider the first term

$$\{\eth_q f, g\}[\eth_p h - \mathrm{Aut}(\eth_p h)] \xrightarrow{\lim} \{\eth_q f, g\} \cdot 0 = 0,$$

and similarly for the other terms. We have already seen that skew-symmetric matrices define almost-Poisson brackets. Now we place an extra condition on these matrices in order to be structure matrices of true Poisson brackets.

Proposition 3. *Consider matrices $J(z) = J^{ij}(z)$ with the properties of a discrete Poisson tensor as in definition* 25. *Then $J(z)$ is a structure matrix for a Poisson bracket if it satisfies the following modified Jacobi identity:*

$$\sum_l \{J^{il}\eth_l J^{jk} + J^{kl}\eth_l J^{ij} + J^{jl}\eth_l J^{ki}\} = 0. \tag{17}$$

Proof. See [12]. □

Remark 3. *(Hamiltonian dynamics on Poisson manifolds.)* We have a canonical mapping from the algebra $A(\mathcal{Z})$ onto the space of discrete vector fields $\mathfrak{X}(A)$ of the algebra

$$f \mapsto X_f = \{f, \cdot\}, \quad \forall f \in A(\mathcal{Z}). \tag{18}$$

This means that our system is represented by the algebra $A(\mathcal{Z})$ which denotes the positions of the system; moreover the algebra is endowed with a canonical mapping $A(\mathcal{Z}) \to \mathfrak{X}(A)$. The dynamics in the smooth case are given by the equations governing the flow of X_H and are called as Hamiltons equations for the Hamiltonian function H. The discrete dynamics are defined as: For any $f \in A(\mathcal{Z})$,

$$\frac{\Delta f(t)}{\Delta t} = \{f, H\} \Rightarrow f_{n+\delta} = f_n + \delta X_H(f_n). \tag{19}$$

So in the limit as $\delta \to 0$ we recover the definition of dynamics in the smooth case $\dot{f} = \{H, f\} = X_H(f)$. The discrete dynamics, as we defined above, gives a mapping $A_n \to A_{n+\delta}$, and this is the algorithm we desire.

The form of equation (19) is very special. Indeed, it implies energy conservation, i.e.

$$\frac{\Delta H}{\Delta t} = \{H, H\} = 0.$$

However most integration techniques are, in general, *not* energy-conserving, and we will see that the above equations actually do not conserve energy.

This would necessitate a modification of the definition of the dynamics (19). For our purposes energy conservation is very important; indeed in future work we aim at extending the discrete framework developed in this paper to port-Hamiltonian systems [22, 23], and then energy conservation is certainly the most important first integral that needs to be conserved. In our definition of discrete Poisson dynamics (19), we assume that we have integration algorithms which are energy-conserving. In example 6, we present one such energy-conserving algorithm, and we also show that energy-conserving algorithms do necessitate a change in the Poisson structure.

6.3. Examples

We have presented a discrete approach towards the modelling of physical systems in this paper. Our claim is that we have presented a framework in which one can formally study discrete systems (whether these discrete models have been obtained as a result of a discretization or by directly doing some form of discrete modelling)—to validate this claim we compare how the simulation results from our discrete models compare with the simulation results of usual discretizations. Moreover the way we have defined our discrete dynamics directly imply energy conservation, and we have to show this in our simulations.

First we do the former, i.e. we take an example of a nonlinear simple pendulum and we compare how, with the choice of a Euler discrete vector, our results correspond to the discretized

results of the pendulum model with the choice of an Euler forward difference technique. In principle, they should not be very different.

Example 5. Consider a simple nonlinear pendulum, whose discrete Hamiltonian function is given by:

$$H(\theta, \dot{\theta}) = \frac{\dot{\theta}^2}{2} - \cos\,\theta,$$

where we assumed, for simplicity, that the length of the pendulum, the mass of the pendulum and gravity are all unity. Then the discrete Hamiltonian dynamics are, using the same Poisson bracket as in example 4,

$$\frac{\Delta\theta}{\Delta t} = \eth_{\dot{\theta}} H(\theta, \dot{\theta}) = \eth_{\dot{\theta}}\left(\frac{\dot{\theta}^2}{2}\right) = \frac{1}{2} \cdot \frac{(\dot{\theta} + h)^2 - \dot{\theta}^2}{h} = \dot{\theta} + \frac{h}{2},$$

$$\frac{\Delta\dot{\theta}}{\Delta t} = -\eth_{\theta} H(\theta, \dot{\theta}) = -\eth_{\theta}(-\cos\theta) = \frac{\cos(\theta + h) - \cos\theta}{\epsilon}$$

$$= \frac{\cos\theta\cos h - \sin\theta\,\sin h - \cos\theta}{h}.$$

This can be rewritten as

$$\begin{bmatrix} \dfrac{\theta(t+\delta) - \theta(t)}{\delta} \\ \dfrac{\dot{\theta}(t+\delta) - \dot{\theta}(t)}{\delta} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \dfrac{\cos\theta\cos h - \sin\theta\,\sin h - \cos\theta}{h} \\ \dot{\theta} + h/2 \end{bmatrix},$$

where h is as defined in (7). The dynamics above look very different from the dynamics that we would obtain by an usual Euler-forward difference discretization technique. The basic difference is in the term ϵ which is present in our model because our spatial domain is also discrete. Indeed, if in the usual discretization schemes the space is also discretized—then one would obtain exactly the same dynamics as above. If we consider the continuum limit for the spatial domain, i.e. $\epsilon \to 0$, then we do recover the usual discretization dynamics. But how do the dynamics as computed in the above equations match with that computed via a usual Euler forward difference discretization method? The answer is—very well! Indeed, as we can see from figure 2 (where we compare θ and $\dot{\theta}$ of both approaches), the matching seems perfect. Actually there is a slight error—for a step size of 0.001 we have found an error of magnitude 10^{-16}, which is indeed extremely good. In other words, we have set up a framework for discrete mechanics that (almost) exactly agrees with the results of a discretization of a smooth physical model[9].

One can see from figure 2 that using an Euler discrete vector the dynamics eventually blow up and this is directly linked to the fact that energy is not conserved in the discrete dynamic evolution. But our formal definition of Poisson dynamics (19) assumes energy conservation. So we must either come up with an algorithm that is energy-conserving, or we must modify our definition of Poisson brackets. In reality, we will need to do both (since some algorithms are energy-conserving and some are not). Below we show how the Euler 'algorithm' can be modified so as to conserve the energy.

[9] Similarly we can show that we have (almost) exactly matching dynamics if we choose, say, Runge–Kutta vectors or Leapfrog vectors, etc.

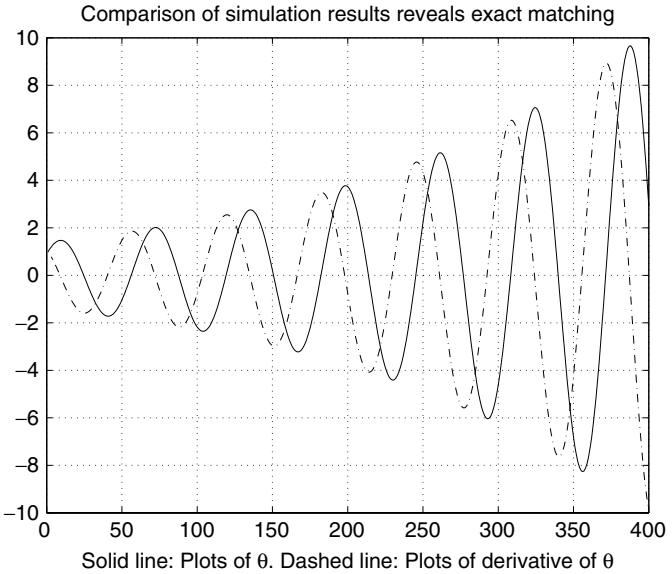

Figure 2. Simulation of a nonlinear pendulum.

Example 6. Consider a discrete model of a linear LC circuit where we assume that $L = C = 1$, the Hamiltonian will have the form $H(q, \phi) = \frac{1}{2}(q^2 + \phi^2)$, where $q(t), \phi(t)$ are discrete curves on a discrete manifold $\mathcal{Z}$. First we consider the usual Euler discrete vector, then we have Hamiltonian dynamics as, using the Poisson bracket of example 4,

$$\frac{\Delta q(t)}{\Delta t} = \frac{q(t+\delta) - q(t)}{\delta} = \eth_{\phi} H(q, \phi) = \eth_{\phi}\left(\frac{\phi^2}{2}\right) = \phi(t) + \frac{h}{2},$$

$$\frac{\Delta \phi(t)}{\Delta t} = \frac{\phi(t+\delta) - \phi(t)}{\delta} = -\eth_{q} H(q, \phi) = -\eth_{q}\left(\frac{q^2}{2}\right) = -q(t) - \frac{h}{2},$$

where h is as defined in (7). Then the energies at times t and $t + \delta$ are given by

$$H(t) = \tfrac{1}{2}(q^2(t) + \phi^2(t)),$$

$$H(t+\delta) = \tfrac{1}{2}([q(t) + \delta \cdot (\phi(t) + h/2)]^2 + [\phi(t) - \delta \cdot (q(t) + h/2)]^2).$$

Obviously $H(t + \delta) \neq H(t)$. There are many ways of exactly conserving energy; cf [3, 5] and the references therein. Now we introduce an Euler integration technique that does conserve energy. The basic idea is adopted from [5], where it was used for non Hamiltonian systems. Consider the modified Euler dynamics:

$$q(t+\delta) = q(t) + \delta \cdot (\phi(t) + h/2), \qquad \phi(t+\delta) = \phi(t) - \delta \cdot ((q(t) + h/2) + f(t)),$$

where $f(t)$ is s.t. $H(t + \delta) - H(t) = 0$ and $f(t) \to 0$ in the continuum limit, such an $f(t)$ is quite easy to obtain. For details of the design of $f(t)$ refer to [5, 12], although in [5] the authors consider non-Hamiltonian systems; the same analysis applies for Hamiltonian systems also. The simulation results are shown in figure 3.

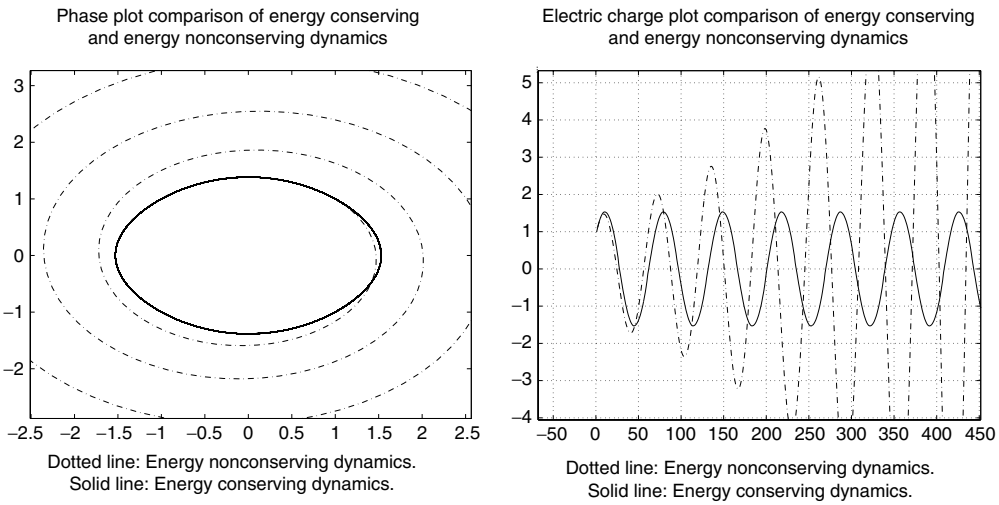

Figure 3. Simulation of a linear LC circuit.

Remark 4. There is however a fundamental problem with the above 'design'. From a geometric viewpoint, what is the meaning of the $f(t)$ term? How does it affect the Poisson structure? From a Hamiltonian framework perspective, it does not make any 'geometric' sense to just add a term to the dynamics[10]. The only thing that one can do in this situation is to make the $f(t)$ term a part of the Poisson structure. In other words, we take $f(t)$ inside the Poisson matrix, so we obtain

$$\begin{bmatrix} \dfrac{q(t+\delta)-q(t)}{\delta} \\ \dfrac{\phi(t+\delta)-\phi(t)}{\delta} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1+\dfrac{f(t)}{q(t)+h/2} & 0 \end{bmatrix} \begin{bmatrix} q(t)+h/2 \\ \phi(t)+h/2 \end{bmatrix}.$$

This however, in general, implies that the modified Poisson structure would lose its basic skew-symmetry property, and this certainly has nontrivial consequences. The only way, which we can think of, to come out of this difficulty is to use the following argument: if in the smooth setting the skew-symmetry ensures energy conservation, in the discrete setting it is the nonskewness that ensures energy conservation!. And mathematically this would make sense, and also since in the continuum limit $f(t) \to 0$ so we recover the usual classical interpretations—this does seem to be a valid argument. However, losing the skewness of the structure has many nontrivial consequences, and one would have to investigate the whole of Hamiltonian mechanics in this modified Poisson framework. In any case, if we do adopt the above argument then one would have to redefine the Poisson dynamics (19) as follows. For any $g \in A(\mathcal{Z})$,

$$\frac{\Delta g(t)}{\Delta t} = \{g, H\} + f(t) \Rightarrow g_{n+\delta} = g_n + \delta X_H(g_n) + \delta f(t), \tag{20}$$

where $f(t)$ is s.t. the discrete energy is conserved, and $f(t) \to 0$ in the limit. That is one option. There is another one—this is what are called port-Hamiltonian systems; see [22–24] and the

[10] Note that this argument holds for other energy-conserving techniques as well.

references therein. In this framework, we can prove that such problems do not exist and we can give a new interpretation and a new (and more useful) geometric structure for discrete Hamiltonian systems. This work is in progress at the moment [11].

7. Conclusions and future work

This paper explores the structure of discrete models of physical systems as to whether these models are obtained through a process of discretization or via directly modelling at the discrete level. To this end we bring together concepts from algebraic geometry (twisted derivations, Kähler differentials), from simplicial homology (which we used to define discrete differential forms), from computer science (floating-point spaces), from numerical analysis (various integration techniques) to define a discrete calculus and a discrete differential geometry on discrete manifolds and finally from noncommutative geometry (to use a tangent groupoid on a smooth manifold for the continuum limit analysis of our discrete models). The next step has been to define discrete dynamics in the Hamiltonian framework, and more specifically on discrete Poisson manifolds. Here again the concept of a twisted derivation plays a fundamental role. Finally we present two examples—the first example shows how we arrive at (almost) exactly the same dynamical behaviour (in the simulations) using our discrete modelling framework, as what we obtain with the usual discretization process. The second example explores some of the implications of energy conservation on the geometric structure of the system. Much more work needs to be done in this regard. We need to formally understand how the geometric structure gets modified if we implement structure-preserving (energy, symplectic structure, Poisson structure, momentum maps etc) properties.

As regarding future work our main interest lies in the subject of port-Hamiltonian systems. Port-Hamiltonian systems are a generalization of Hamiltonian systems—instead of the usual Poisson (or symplectic) structure one uses a more general structure called the *Dirac structure*. The basic goal of this framework is to treat complex systems as an *interconnection* of simpler subsystems (allowing for energy flow between the interconnected subsystems), and the interconnection structure is formalized by a Dirac structure. So the modelling of dissipative phenomena, for example, is very natural in this framework. This modelling framework is quite important, both from a theoretical viewpoint and a technological viewpoint. There are two motivations for extending the framework of this paper to port-Hamiltonian systems. The first one is basically the motivations given for this paper, in that we are interested in understanding the structure of discrete port-Hamiltonian systems, and to model interconnected systems directly at a discrete level, so as to facilitate trivial computer implementations for numerical simulation. The other goal is actually more fundamental, and useful. We have seen the fundamental problems involved with discrete Hamiltonian systems (whether obtained via a discretization process or via directly modelling at the discrete level)—in general they do not have important conservation properties (energy, symplectic/Poisson, momentum maps, etc). Now, it can be shown [11] that discrete Hamiltonian systems are a special case of discrete-port-Hamiltonian systems. One advantage of this is that the addition of various (energy, Poisson, etc) conserving techniques can be given a clear and precise geometric formalism. As we have seen in example 6, the addition of the f term is quite difficult to interpret in the Hamiltonian (i.e. Poisson structure) framework; it is nothing more than an interconnecting variable in the port-Hamiltonian (i.e. Dirac structure) framework, in other words it is an interconnecting variable. And, more importantly, this would imply that numerical simulation problems can be treated as control theoretic (cf [25, 26]), problems, and this would be a common meeting ground for modelling, numerical simulation and control theory.

Another aspect that we would like to study is the extension of this theory to infinite-dimensional systems. The present paper concerns only finite-dimensional systems, so the natural extension would be to infinite-dimensional systems. This will be the focus of our future work.

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